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LASER SPECTROSCOPY OF TRANSIENT MOLECULES IMPORTANT IN
EXPLOSIONS(U) ARIZONA UNIV TUCSON DEPT OF CHEMISTRY
P F BERNATH 20 MAR 87 N00014-84-K-0012

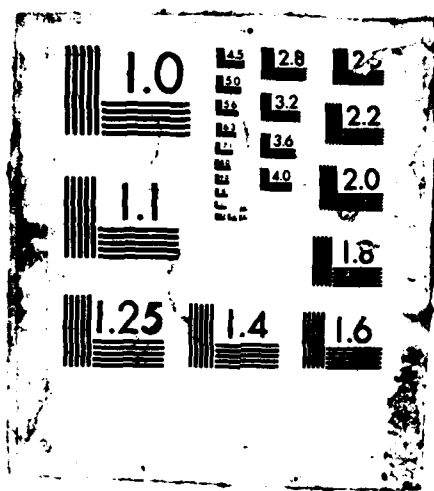
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We have observed the high-resolution Fourier transform spectra of the NH , CH , Mg , NaH , CaH , Ca^+ and Ba molecules. The technique of Fourier transform detection of laser-induced fluorescence was applied to free radicals in order to simplify the complex emission spectrum of CCN . A free radical jet source was utilized with a Fourier transform spectrometer to obtain the ultracold emission spectrum of CH^+N and CD^+N . A large number of metal-containing free radicals such as CaNCO , CaNNN , CaC_5H_5^+ and CaOR were discovered by laser-induced fluorescence.

(keywords: Calcium nitracarbonate)

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A. Fourier Transform Spectroscopy of Free Radicals

The McMath Fourier transform spectrometer was used to record the high-resolution emission spectra of many transient species.

1. NH

The NH radical is one of the simplest and most important species thought to occur in detonations. The $A^3\Pi-X^3\Sigma^-(4)$ and $c^1\Pi-a^1\Delta$ (5) electronic transitions were recorded in the ultraviolet region of the spectrum.

2. CH

The vibration-rotation spectrum of the ground $X^2\Pi$ state of the CH radical was recorded in the infrared (9). The excited vibrational levels with $v=2$ and 3 were characterized for the first time. These excited levels will certainly be populated in the energetic environment of a detonation.

3. PH

The PH molecule is isovalent with NH. The infrared vibration-rotation spectrum was analyzed (8). Phosphorous compounds have many military applications from chemical warfare agents to grenades.

4. CP

The CP free radical is isovalent with the CN radical. The $A^2\Pi-X^2\Sigma^+$ electronic transition (7) was observed for the first time. This transition corresponds to the red system of CN occurs in the infrared for CP.



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5. MgH, NeH⁺ and CuH

The visible $A^2\Pi-X^2\Sigma^+$ spectrum of MgH (1) and the vibration-rotation spectra of NeH⁺ (2) and CuH (3) were observed with partial ONR support. These molecules are of astrophysical importance (MgH and CuH are found in the sun) or of potential astrophysical interest (NeH⁺ may be found in planetary nebulae).

6. CCN

The technique of Fourier transform detection of laser-induced fluorescence was applied to free radicals for the first time. Five bands of the $A^2\Delta-X^2\Pi$ transition of CCN were detected (6). This technique has great promise for the simplification of complex polyatomic emission spectra.

7. CH₃N and CD₃N

An Engelking type of free radical jet source was used to observe the ultracold emission spectrum of CH₃N and CD₃N (10). Our work represents the first high-resolution study of this radical. Without the simplification provided by the low rotational temperatures of our source, the spectrum would be much too complicated to analyze. The CH₃N work illustrates the power of combining a radical jet source with modern Fourier transform methods of detection.

8. Metal cyanates, azides, alkoxides and cyclopentadienides

We have discovered a large number of novel metal (Ca and Sr)-containing free radicals with partial ONR support (11-14). These molecules include CaNCO, SrNCO, CaNNN, SrNNN, CaC₅H₅, SrC₅H₅, CaOR and SrOR (R=CH₃, CH₂CH₃, etc.). The electronic, vibrational and, in favorable cases, rotational structures

were determined by laser-induced fluorescence. Metal azides are used as detonators. Our discovery of the CaNNN and SrNNN molecules represents the first observation of a gas-phase metal azide.

FINAL REPORT

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